

Coherent molecular bound states of bosons and fermions near a Feshbach resonance

P. D. Drummond and K. V. Kheruntsyan

ARC Centre of Excellence for Quantum-Atom Optics, Department of Physics,
University of Queensland, Brisbane, Qld 4072, Australia

(Dated: February 2, 2008)

We analyze molecular bound states of atomic quantum gases near a Feshbach resonance. A simple, renormalizable field theoretic model is shown to have exact solutions in the two-body sector, whose binding energy agrees well with observed experimental results in both Bosonic and Fermionic cases. These solutions, which interpolate between BEC and BCS theories, also provide a more general variational ansatz for resonant superfluidity and related problems.

PACS numbers: 03.75.Nt, 05.30.-d, 39.25.+k, 67.40.-w

The coherent transformation of a cold atomic gas to molecules in the vicinity of a photoassociation [1] or Feshbach [2] resonance has enabled a fascinating probe of quantum dynamical behavior in coupled atom-molecular systems, together with remarkably precise measurements of quantum binding energies. Recent Bosonic experiments have extended the available species to ^{133}Cs , ^{87}Rb , and ^{23}Na [3]. Experiments on ultracold degenerate Fermi gases of ^{40}K and ^6Li atoms have resulted in spectacular demonstrations of molecular Bose-Einstein condensate (BEC) formation [4, 5] and of possible fermion superfluid behavior in the BEC-BCS crossover region [6].

Since these are many-body systems, it is useful to try to develop the simplest possible field-theoretic model that can explain their behavior. An essential feature of any correct many-body treatment is that the basic theory must be able to reproduce the physics of the two-body interactions. In this paper, we combine previous analytic solutions of a coherently coupled field theory [7, 8, 9] with an exact renormalization of the coupling constants [10], in order to obtain analytic predictions for the two-body bound states. This gives a unified picture of any Feshbach resonance experiment and related studies [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20], provided a small number of observable parameters are available. The predictions will be compared with experimental data and with coupled-channel calculations.

To quantitatively model these experiments, consider an effective Hamiltonian for the molecular field ($\hat{\Psi}_0$) in the closed channel and the atomic fields ($\hat{\Psi}_{1(2)}$) in the free-atom dissociation limit of the open channel:

$$\hat{H}_1 = \hat{H}_0 + \frac{\hbar}{2} \int d^3\mathbf{x} \sum_{i,j} U_{ij} \hat{\Psi}_i^\dagger \hat{\Psi}_j^\dagger \hat{\Psi}_j \hat{\Psi}_i, \quad (1)$$

with the commutation (+) or anti-commutation (-) relation $[\hat{\Psi}_i(\mathbf{x}, t), \hat{\Psi}_j^\dagger(\mathbf{x}', t)]_\pm = \delta_{ij} \delta(\mathbf{x} - \mathbf{x}')$ for Bosonic or Fermionic field operators $\hat{\Psi}_i$, respectively. The free Hamiltonian \hat{H}_0 includes the usual kinetic energy terms and the potential energies (including internal energies) due to the trap potential $\hbar V_i(x)$, while U_{ij} is the atom-atom, atom-molecule, and molecule-molecule coupling due to s -wave scattering. The atomic and molecular masses are $m_{1,2}$ and $m_0 = m_1 + m_2$, and $E_m =$

$\hbar[V_0(0) - V_1(0) - V_2(0)]$ gives the bare energy detuning of the molecular state with respect to free atoms.

Next, we consider a coherent process of Raman photoassociation or a magnetic Feshbach resonance coupling, giving rise to an overall effective Hamiltonian term in the homonuclear case (only with bosons) [7, 8]

$$\hat{H} = \hat{H}_1 + \frac{\hbar\chi}{2} \int d^3\mathbf{x} [\hat{\Psi}_0^\dagger \hat{\Psi}_1^2 + \hat{\Psi}_1^{\dagger 2} \hat{\Psi}_0], \quad (2)$$

or, for the case of heteronuclear dimer formation involving either fermions or bosons [9]:

$$\hat{H} = \hat{H}_1 + \hbar\chi \int d^3\mathbf{x} [\hat{\Psi}_0^\dagger \hat{\Psi}_1 \hat{\Psi}_2 + \hat{\Psi}_2^\dagger \hat{\Psi}_1^\dagger \hat{\Psi}_0]. \quad (3)$$

Here, χ is the bare atom-molecule coupling responsible for the conversion of free atom pairs into molecules and vice versa. The heteronuclear case can be applied to Fermionic atom pairs in different spin states ($\hat{\Psi}_1, \hat{\Psi}_2$) combining into a Bosonic molecule ($\hat{\Psi}_0$), or pairs of Bosonic and Fermionic atoms combining into a Fermionic molecule, or else to a fully Bosonic case where the atom pairs are not identical.

Bosonic homonuclear case. First we consider the fully Bosonic uniform case of Eq. (2), i.e., a single-species atomic BEC (with $m_1 \equiv m$) coupled to a molecular BEC, where the atomic background energy is chosen to be zero. We ignore inelastic collisions – which is a reasonable approximation at low density, and let $\kappa = U_{11}$, where κ is the bare atom-atom coupling due to s -wave scattering.

Here a momentum cutoff is implicitly assumed, since in renormalizable theories one expects to obtain finite results only after the infinities are absorbed through a redefinition of bare couplings. To manipulate integrals that *a priori* are divergent, we regularize them by a simple cutoff: integrals over \mathbf{k} are restricted to $|\mathbf{k}| < K$.

The homogeneous Hamiltonian, Eq. (2), has an exact eigenstate in the simplest two-particle sector [7, 8]. In momentum space, we expand the field operators $\hat{\Psi}_0(\mathbf{x})$ and $\hat{\Psi}_1(\mathbf{x})$ in terms of Fourier components $\hat{a}(\mathbf{k})$ and $\hat{b}(\mathbf{k})$, respectively, with commutation relations $[\hat{a}(\mathbf{k}), \hat{a}^\dagger(\mathbf{k}')] = [\hat{b}(\mathbf{k}), \hat{b}^\dagger(\mathbf{k}')] = \delta(\mathbf{k} - \mathbf{k}')$. Including a cutoff K , the (unnormalized) two-particle eigenstate corresponding to the

zero center-of-mass momentum is given by [7, 8]

$$|\Psi^{(N)}\rangle = \left[\hat{a}^\dagger(0) + \int_{|\mathbf{k}|=0}^K \frac{d^3\mathbf{k} G(\mathbf{k})}{(2\pi)^{3/2}} \hat{b}^\dagger(\mathbf{k}) \hat{b}^\dagger(-\mathbf{k}) \right]^{N/2} |0\rangle, \quad (4)$$

where $N = 2$ in the exactly soluble two-particle case, and $G(\mathbf{k})$ is the atomic pair correlation function in Fourier space. This coherent superposition of a molecule with correlated pairs of atoms can be viewed as a dressed molecule. More generally, this is also a useful low-density variational ansatz for $N > 2$ particles, where it describes a BEC of dressed molecules [7, 8].

Fermionic or heteronuclear case. Next, we wish to consider the important case of Fermionic atom pairs (with $m_1 = m_2 \equiv m$) in different spin states combining into a Bosonic molecule. This is especially relevant to the studies of ultracold Fermi gases [4, 5, 6] in the region of resonant superfluidity and BEC-BCS crossover. These experiments are notable for the greatly reduced inelastic loss rate from atom-molecular collisions, due to Pauli blocking [22]. In this Fermionic case, we only have an s -wave coupling between the different fermions, so that $\kappa = U_{12}$. In addition, the final results of this section can be applied to heteronuclear molecules (with either statistics of the constituent atoms), except that the mass m has to be replaced by $2m_r$, where $m_r = m_1 m_2 / (m_1 + m_2)$ is the reduced mass.

The Hamiltonian (3) relevant to this case, also has an exact eigenstate in the two-particle ($N = 2$) sector [9]. Expanding the field operators $\hat{\Psi}_{1,2}(\mathbf{x})$ in terms of Fourier components $\hat{b}_{1,2}(\mathbf{k})$, the eigenstate is now given by

$$|\Psi^{(N)}\rangle = \left[\hat{a}^\dagger(0) + \int_{|\mathbf{k}|=0}^K \frac{d^3\mathbf{k} G(\mathbf{k})}{(2\pi)^{3/2}} \hat{b}_1^\dagger(\mathbf{k}) \hat{b}_2^\dagger(-\mathbf{k}) \right]^{N/2} |0\rangle. \quad (5)$$

As before, this is also a useful variational ansatz for the N -particle ($N > 2$) ground state, where it extends BCS theory to include a coherent molecular field.

Exact eigenvalues. In either the homonuclear or heteronuclear case, the exact energy eigenvalue corresponding to the two-particle eigenstate ($N = 2$) is known [8, 9]. Introducing a multiplicity parameter s , where $s = 1$ for the homonuclear case, and $s = 2$ for the Fermionic or heteronuclear case, we find that

$$E = E_m - \frac{\hbar s \chi^2}{2} \left[\kappa + \frac{2\pi^2 \hbar r_0 / m}{r_0 K - \tan^{-1}(r_0 K)} \right]^{-1} = -\frac{\hbar^2}{m r_0^2}. \quad (6)$$

For real and positive r_0 , this corresponds to a bound state with negative energy, and the resulting binding energy is $E_b = -E$. The quantity r_0 is the correlation radius or the effective size of the dressed molecule. The right-hand side of Eq. (6) needs to be solved for r_0 , or equivalently for the binding energy $E_b \equiv \hbar^2 / (m r_0^2)$ as a function of E_m , but in general it has no explicit solution.

Next, it is useful to re-express the bare Hamiltonian parameters in terms of renormalized observable parameters that are invariant at large momentum cutoff. We therefore include a nonperturbative renormalization using integral equation methods from scattering theory [10], which has some subtle features. In particular, a repulsive contact potential with $\kappa > 0$ has no effect – it does not lead to scattering in three-dimensional field theory. However, either positive or negative scattering lengths can be generated from the same type of attractive contact potential with $\kappa < 0$, depending on the limiting procedure: if it is carried out with sufficiently deep potentials to allow a bound state to form in the atomic field channel, then a positive scattering length is possible even with an attractive short-range potential.

The renormalization [10] expresses the bare values as $\kappa = \Gamma \kappa_0$, $\chi = \Gamma \chi_0$, and $E_m = E_0 + s \hbar \beta \Gamma \chi_0^2 / 2$, in terms of the observed or renormalized values κ_0 , χ_0 , and E_0 . In the Feshbach resonance case, for definiteness, $E_0 = \Delta \mu (B - B_0)$. Here, the cutoff K is included through a scaling parameter $\Gamma = (1 - \beta \kappa_0)^{-1}$, where $\beta = m K / (2\pi^2 \hbar)$, $\kappa_0 = 4\pi \hbar a_{bg} / m$, and a_{bg} is the background s -wave scattering length for the atoms. In the homonuclear case, $\Delta \mu = 2\mu_1 - \mu_m$ is the magnetic moment difference between the atomic and the bound molecular channels, and B_0 is the magnetic field corresponding to the resonance, while in the heteronuclear case, $\Delta \mu = \mu_1 + \mu_2 - \mu_m$.

We now wish to rewrite Eq. (6) in terms of the renormalized constants χ_0 , κ_0 , and E_0 . After taking the limit of large momentum cutoff K , we obtain the following simple analytic result:

$$E_0 = -E_b - \frac{s C \hbar \chi_0^2 \sqrt{E_b}}{1 - 2C \kappa_0 \sqrt{E_b}}, \quad (7)$$

where $C \equiv m^{3/2} / (8\pi \hbar^2)$. Using $E_0 = \Delta \mu (B - B_0)$, Eq. (7) can also be rewritten in terms of the magnetic fields, so that the resulting binding energy can be directly compared with the experimental data.

In the JILA ^{85}Rb experiments [2, 21], the creation of a homonuclear dressed molecular state at a given B value is followed by a rapid change in the magnetic field which allows an interference fringe to be observed in the remaining total number of atoms. The reason for the fringe is due to the fact that in a dynamical experiment, paired atoms in the dressed molecular wave function can interfere constructively or destructively with condensate atoms that are not in the ground-state wave function. The resulting interference pattern oscillates with a frequency corresponding to the dressed molecular binding energy.

A graphical solution of Eq. (7), i.e., the binding energy E_b vs B for the JILA ^{85}Rb experiment [2, 21], is plotted in Fig. 1, together with experimentally observed Ramsey fringe frequencies, which are interpreted in the

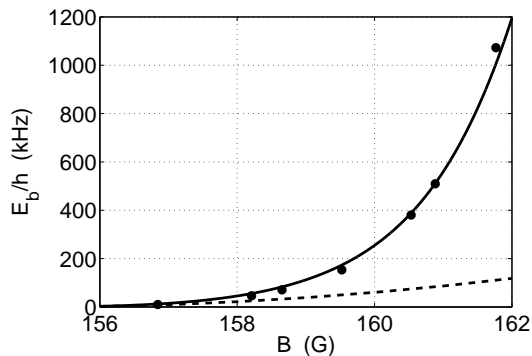


FIG. 1: Binding energy E_b versus the magnetic field B for the ^{85}Rb experiment [2]. The parameter values are taken from the subsequent high-precision measurements on the same system [21]: $B_0 = 155$ G and $a_{bg} = -443a_0$, where a_0 is the Bohr radius. In addition, we take $\chi_0 = 2.84 \times 10^{-4} \text{ m}^{3/2}/\text{s}$ and $\Delta\mu = -2.23\mu_B$ [23], where μ_B is the Bohr magneton. The solid line is our theoretical result, Eq. (7), while the dashed line is the result of Eq. (8). The circles are the experimental data of Ref. [21].

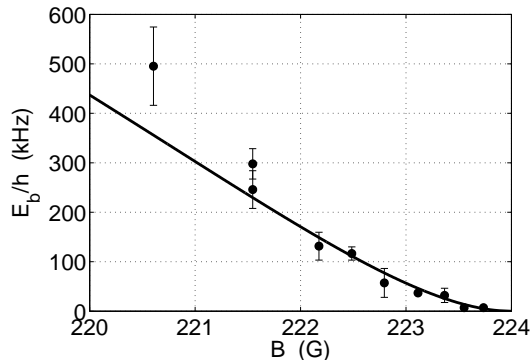


FIG. 2: Binding energy E_b vs B for the ^{40}K experiment [4], where $B_0 = 224$ G and $a_{bg} = 174a_0$. In addition, we take $\chi_0 = 1.12 \times 10^{-4} \text{ m}^{3/2}/\text{s}$ and $\Delta\mu = 1.27\mu_B$ [23]. The solid line is our theoretical result, while the circles and the error bars are the experimental data from Fig. 5 of Ref. [4].

experiment as a dressed molecular binding energy. The agreement between this simple analytic result and the experimentally observed binding energy (as well as the coupled-channel calculation [10]) is excellent.

Binding energy measurements were also carried out for the case of Fermionic ^{40}K atoms in two different spin states combining into a Bosonic molecule [4]. In Fig. 2 we plot the solution to Eq. (7), i.e., the binding energy E_b vs the magnetic field B , for this experiment, where we also see a good agreement between the theory and experiment.

Near-threshold physics. There are common features with either Fermionic and Bosonic atoms. All results are expressed in terms of the four observable parameters χ_0 , κ_0 , $\Delta\mu$, B_0 , and are clearly independent of the cutoff, as

one would expect from a renormalizable theory. There are two cases corresponding to different signs of κ_0 :

- (i) Attractive case. If $a_{bg} < 0$, then E_b is a single-valued function of B , so there is only one solution branch.
- (ii) Repulsive case. If $a_{bg} > 0$, then E_b is a double-valued function of B , so there are two solution branches. This case has a bound state in the atomic channel.

In all cases, the physics near threshold is crucial to understanding either type of experiment. For small binding energies in the vicinity of the resonance, Eq. (7) gives a quadratic dependence of E_b on E_0 (or on the magnetic field B): $E_b \simeq E_0^2 / (sC\hbar\chi_0^2)^2$, where $E_0 = \Delta\mu(B - B_0)$. This is in agreement with the simple resonant scattering theory result that $E_b = \hbar^2/ma(B)^2$ near the resonance [18, 24]. Here, the effective scattering length is $a(B) = a_{bg} [1 - \Delta B / (B - B_0)]$, ΔB is the width of the resonance, and the atom-molecule coupling χ_0 can be expressed via ΔB as follows: $\chi_0 \simeq \sqrt{8\pi a_{bg} \Delta\mu \Delta B / (sm)}$.

In the opposite limit of large E_b , i.e., for magnetic fields far away from the resonance, the same equation (7) gives linear dependence of E_b on E_0 (and hence on B) as expected, $E_b \simeq -E_0 + s\hbar\chi_0^2/(2\kappa_0)$, including a constant energy shift. This linear behavior is not accessible with the resonant scattering theory result of $E_b = \hbar^2/ma(B)^2$.

For $C|\kappa_0|\sqrt{E_b} \ll 1$, i.e., either for small background scattering $|a_{bg}|$ or small binding energies E_b near the resonance, we can neglect $2C\kappa_0\sqrt{E_b}$ in the denominator of the second term in Eq. (7) and obtain a quadratic with respect to $\sqrt{E_b}$. This has the following explicit solution:

$$E_b \simeq -E_0 - \frac{(sC\hbar\chi_0^2)^2}{2} \left[\sqrt{1 - \frac{4E_0}{(sC\hbar\chi_0^2)^2}} - 1 \right], \quad (8)$$

which (for $s = 1$) coincides with Eq. (21) of Ref. [17]. This result formally incorporates the above-mentioned quadratic dependence of E_b on E_0 near the resonance where $4E_0/(sC\hbar\chi_0^2)^2 \ll 1$, and the linear dependence far away from the resonance. The quadratic dependence is in qualitative agreement with the behavior found from our exact result. However, the linear part ($E_b \simeq -E_0$) – while giving the correct slope of the binding energy – does not account for the energy shift term $s\hbar\chi_0^2/(2\kappa_0)$ due to the renormalization of E_m . This leads to a discrepancy seen in Fig. 1 (dashed line) away from the resonance, and is due to the fact that the assumption of $C|\kappa_0|\sqrt{E_b} \ll 1$ used to obtain Eq. (8) is inconsistent with the case of large binding energies under consideration. We note here that it is also possible to obtain the exact result from the molecular Green's function method of Ref. [17], if the relevant self-energy term is included without approximation [25].

The relative fraction of the atomic and molecular components in the two-particle eigenstate can be calculated using the conserved total number of atomic particles, $\hat{N} = \hat{N}_1 + 2\hat{N}_0$ (or $\hat{N} = \hat{N}_1 + \hat{N}_2 + 2\hat{N}_0$ in the Fermionic

case). At low density, the closed-channel molecular fraction is (including a factor of 2 to reflect the fact that each molecule consists of two atoms):

$$2N_0/N = (1 + 2F/s)^{-1}. \quad (9)$$

Here, $F \equiv \int d^3\mathbf{k} G^2(\mathbf{k})/(2\pi)^3$, and the correlation function $G(\mathbf{k})$ is given by a Lorentzian

$$G(\mathbf{k}) = G_0 / (1 + r_0^2 k^2), \quad (10)$$

where $k = |\mathbf{k}|$, $G_0 = sm\chi_0 r_0^3/[2\hbar(a_{bg} - r_0)]$, and we have already taken into account renormalization. Taking the integral in F we obtain that

$$F = \frac{G_0^2}{8\pi r_0^3} = \frac{s^2 m^{3/2} \chi_0^2}{32\pi\hbar\sqrt{E_b}} \left(1 - \frac{m^{3/2}\kappa_0}{4\pi\hbar^2} \sqrt{E_b}\right)^{-2}, \quad (11)$$

where we have expressed $r_0 = \hbar/\sqrt{mE_b}$, so that the final result can be analyzed as a function of the magnetic field B using the solution to Eq. (7).

Combining this result with Eqs. (7) and (9), we find that the average fraction of bare molecules in the closed channel is typically very small near the resonance. For example, for ^{85}Rb parameters [21] it is no higher than $2N_0/N \simeq 0.07$, for magnetic fields from B_0 to $B \simeq 160$ G. This implies that the structure of the dressed molecules and the underlying physics near the resonance is dominated by the correlated atom pairs rather than by the closed channel molecules.

We can also calculate the atomic pair correlation in coordinate space. This is the inverse Fourier transform of $G(\mathbf{k})$ given by $g(\mathbf{x}) = G_0 \exp(-|\mathbf{x}|/r_0)/(2\pi r_0^2 |\mathbf{x}|)$, for $|\mathbf{x}| > 0$. Since $r_0 = \hbar/\sqrt{mE_b}$, it is clear that, near threshold, the bound states are superpositions of molecules with pairs of atoms at very long range. Here, one can expect modifications [18] of the binding energy due to mean-field many-body interactions of the correlated atoms, which have a character similar to Cooper pairs. Such departures from the predicted binding energies are indeed observed [21] in high-precision Ramsey spectroscopy for ^{85}Rb . Similarly, recent collective-mode spectroscopy in ^6Li has revealed BCS-like behavior near threshold with reduced mode frequencies [26], quite different to that expected for a conventional molecular BEC.

In summary, a relatively simple field-theoretic model for Feshbach coupling has exact solutions for the eigenstates in the low-density two-particle sector. It is able to accurately predict Feshbach dressed-molecule binding energies, and also gives a physical understanding of the type of correlated atom-molecular structure produced in these experiments. The model has a simple, universal character, and can be used to describe a variety of cases with both positive and negative background scattering length. Having analytic solutions of the actual eigenstates provides an alternative picture that aids in understanding these interesting experiments, and is readily usable as a starting point to a more complete many-body theory.

The authors gratefully acknowledge the Australian Research Council for the support of this work, and thank M. Holland, C. Pethick, and X.-J. Liu for useful discussions. The research was also supported by the National Science Foundation under Grant No. PHY99-07949.

-
- [1] R. H. Wynar *et al.*, Science **287**, 1016 (2000).
 - [2] E. A. Donley *et al.*, Nature **417**, 529 (2002).
 - [3] J. Herbig *et al.*, Science **301**, 1510 (2003); K. Xu. T. Mukaiyama *et al.*, *ibid.* **91**, 210402 (2003); S. Dürr *et al.*, Phys. Rev. Lett. **92**, 020406 (2004).
 - [4] C. A. Regal *et al.*, Nature **424**, 47 (2003).
 - [5] M. Greiner *et al.*, Nature **426**, 537 (2003); K. E. Strecker *et al.*, Phys. Rev. Lett. **91**, 080406 (2003); J. Cubizolles *et al.*, *ibid.*, 240401 (2003); S. Jochim *et al.*, *ibid.*, 240402 (2003); M. W. Zweirlein *et al.*, *ibid.*, 250401 (2003).
 - [6] C. A. Regal, M. Greiner, and D. S. Jin, Phys. Rev. Lett. **92**, 040403 (2004); M. Bartenstein *et al.*, *ibid.* 120401 (2004); M. W. Zweirlein *et al.*, *ibid.* 120403 (2004).
 - [7] P. D. Drummond, K. V. Kheruntsyan, and H. He, Phys. Rev. Lett. **81**, 3055 (1998).
 - [8] K. V. Kheruntsyan and P. D. Drummond, Phys. Rev. A **58**, R2676 (1998). We use r_0 instead of the μ^{-1} used previously, while E_m corresponds to $\hbar\rho$.
 - [9] K. V. Kheruntsyan and P. D. Drummond, Phys. Rev. A **61**, 063816 (2000).
 - [10] M. Holland *et al.*, Phys. Rev. Lett. **87**, 120406 (2001); S. J. J. M. F. Kokkelmans *et al.*, Phys. Rev. A **65**, 053617 (2002); S. J. J. M. F. Kokkelmans and M. J. Holland, Phys. Rev. Lett. **89**, 180401 (2002).
 - [11] D. J. Heinzen, R. Wynar, P. D. Drummond, and K. V. Kheruntsyan, Phys. Rev. Lett. **84**, 5029 (2000).
 - [12] E. Timmermans *et al.*, Phys. Rep. **315**, 199 (1999); E. Timmermans *et al.*, Phys. Rev. Lett. **83**, 2691 (1999); E. Timmermans *et al.*, Phys. Lett. A **285**, 228 (2001).
 - [13] J. Javanainen and M. Mackie, Phys. Rev. A **59**, R3186 (1999); M. Mackie, K. A. Suominen, and J. Javanainen, Phys. Rev. Lett. **89**, 180403 (2002).
 - [14] F. A. van Abeelen and B. J. Verhaar, Phys. Rev. Lett. **83**, 1550 (1999).
 - [15] V. A. Yurovsky, A. Ben-Reuven, P. S. Julienne, and C. J. Williams, Phys. Rev. A **60**, R765 (1999).
 - [16] K. Góral, M. Gajda, and K. Rzażewski, Phys. Rev. Lett. **86**, 1397 (2001).
 - [17] R. A. Duine and H. T. C. Stoof, J. Opt. B: Quantum Semiclass Opt. **5**, S212 (2003).
 - [18] R. A. Duine and H. T. C. Stoof, cond-mat/0312254.
 - [19] T. Köhler, T. Gasenger, and K. Burnett, Phys. Rev. A **67**, 013601 (2003).
 - [20] G. M. Bruun and C. J. Pethick, Phys. Rev. Lett. **92**, 140404 (2004).
 - [21] N. R. Claussen *et al.*, Phys. Rev. A **67**, 060701 (2003).
 - [22] D. S. Petrov, C. Salomon, and G. V. Shlyapnikov, Phys. Rev. Lett. **93**, 090404 (2004).
 - [23] M. Holland, private communication.
 - [24] J. J. Sakurai, *Modern Quantum Mechanics* (Addison-Wesley, New York, 1994).
 - [25] X.-J. Liu, private communication.
 - [26] M. Bartenstein *et al.*, Phys. Rev. Lett. **92**, 203201 (2004).